

Generalized virial theorem for the Liénard-type systems

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DOI: 10.1007/s12043-014-0925-0; ePublication: 26 February 2015

Abstract. A geometrical description of the virial theorem (VT) of statistical mechanics is presented using the symplectic formalism. The character of the Clausius virial function is determined for second-order differential equations of the Liénard type. The explicit dependence of the virial function on the Jacobi last multiplier is illustrated. The latter displays a dual role, namely, as a position-dependent mass term and as an appropriate measure in the geometrical context.

Keywords. Virial theorem; Liénard-type equation; Jacobi last multiplier; symplectic form; Banach manifold.

PACS Nos 02.40.Yy; 45.20.Jj; 03.65.Ca

1. Introduction

The virial theorem (VT) is an important theorem of classical mechanics which has been successfully applied in the last century to a number of relevant physics problems, mainly in astrophysics, cosmology, molecular physics, quantum mechanics and in statistical mechanics. In mechanics, it provides a general equation relating the average over time of the total kinetic energy, $\langle\langle T \rangle\rangle$, of a stable system consisting of N particles, bound by potential forces, with that of the total potential energy, $\langle\langle V_{\text{TOT}} \rangle\rangle$, where angle brackets represent the average over time of the enclosed quantity. The word virial derives from *vis*, the latin word for force or energy and was introduced by Rudolf Clausius in 1870 [1]. The scalar virial theorem says that kinetic and potential energies must be in balance, whereas the tensor virial theorem [2,3] says that the kinetic and potential energies must be in balance in each separate direction. The scalar theorem is useful for estimating global average property while the tensor virial theorem is useful for relating the shapes of the

system. Recently, Li *et al* [4] considered the hypervirial theorem (HVT) and obtained the hypervirial relations. The HVT and Hellmann–Feynman theorem are shown to provide a powerful method of generating perturbation expansions.

In this paper we consider geometrical mechanics approach and necessity of geometric treatment of VT [5,6] can be argued as follows. The standard VT is based on the transformation properties of kinetic and potential energies under dilations, and therefore is only valid for systems with \mathbb{R}^n as configuration space. In order to generalize the VT for other systems, the tools of geometric mechanics are used.

1.1 Standard approach of virial theorem

Clausius introduced the virial function for a one-particle system

$$G(\mathbf{x}, \dot{\mathbf{x}}) = m\mathbf{x} \cdot \dot{\mathbf{x}} = \frac{d}{dt} \left(\frac{1}{2} m\mathbf{x} \cdot \dot{\mathbf{x}} \right)$$

for studying the motion of a particle of mass m under the action of a force F . The time evolution of G is given by

$$\frac{dG}{dt} = m\dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + \mathbf{x} \cdot \mathbf{F},$$

where we use Newton’s second law, $\mathbf{F} = m\ddot{\mathbf{x}}$.

On integrating this expression between $t = 0$ and $t = T$ and dividing by the total time interval T we find

$$\begin{aligned} \frac{1}{T} [G(T) - G(0)] &= \frac{2}{T} \int_0^T K(\dot{\mathbf{x}}) dt + \frac{1}{T} \int_0^T \mathbf{x} \cdot \mathbf{F} dt \\ &= \langle \langle 2K(\dot{\mathbf{x}}) \rangle \rangle + \langle \langle \mathbf{x} \cdot \mathbf{F} \rangle \rangle, \end{aligned}$$

where $K(\dot{\mathbf{x}}) = \frac{1}{2} m(\dot{\mathbf{x}} \cdot \dot{\mathbf{x}})$ and $\langle \langle A \rangle \rangle$ is the time average. By time average we mean

$$\langle \langle F \rangle \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T F(\mathbf{x}(t)) dt.$$

If either the motion is periodic of period T or the possible values of the function G are bounded, then we take the limit $T \rightarrow \infty$:

$$0 = \langle \langle 2K(\dot{\mathbf{x}}) \rangle \rangle + \langle \langle \mathbf{x} \cdot \mathbf{F} \rangle \rangle.$$

For $F = -\nabla V$, this becomes

$$0 = \langle \langle 2K(\dot{\mathbf{x}}) \rangle \rangle - \langle \langle \mathbf{x} \cdot \nabla V \rangle \rangle.$$

If the potential V is homogeneous of degree k , Euler’s theorem of homogeneous functions implies that $\mathbf{x} \cdot \nabla V = kV$, thus we obtain by

$$\langle \langle 2K(\dot{\mathbf{x}}) \rangle \rangle = k \langle \langle V(\mathbf{x}) \rangle \rangle.$$

If E is the total energy, then

$$\langle \langle K(\dot{\mathbf{x}}) \rangle \rangle = \frac{kE}{k+2}, \quad \langle \langle V(\mathbf{x}) \rangle \rangle = \frac{2E}{k+2}.$$

For harmonic oscillator:

$$\langle \langle K(\dot{\mathbf{x}}) \rangle \rangle = \langle \langle V(\mathbf{x}) \rangle \rangle = \frac{1}{2} E$$

and for Kepler equation

$$\langle \langle K(\dot{\mathbf{x}}) \rangle \rangle = -E, \quad \langle \langle V(\mathbf{x}) \rangle \rangle = 2E.$$

2. Symplectic form, Hamiltonian systems and virial theorem

The pair (M, ω) of a smooth manifold M with a symplectic form ω is called a symplectic manifold. A necessary condition for the existence of a symplectic form ω on M is that M should have even dimension $2n$, so for all practical purposes one can imagine M as a generalized phase space. Throughout this paper we assume that M is a smooth manifold. A Hamiltonian system is a triple (M, ω, H) , where (M, ω) is a symplectic manifold and $H \in C^\infty(M, \mathbb{R})$ is a function, called the Hamiltonian function.

Starting with a Hamiltonian function H , one produces a vector field X_H as follows:

$$H \rightarrow X_H : \omega(X_H, \cdot) = i_{X_H} \omega = dH,$$

which defines a flow ϕ_t on M and the Hamiltonian H is a conserved quantity under this flow. Hamiltonian equations are dynamical systems for the vector field X_H . The Poisson bracket for any two Hamiltonian functions F and H in M is given by

$$\{F, H\} = \omega(X_F, X_H) = X_H F = -X_F H.$$

The flow ϕ_t commutes with X_H for any $w \in C^\infty(M)$

$$X_H \phi_t^* w = \phi_t^* X_H w = \frac{d}{ds} [\phi_s^* (\phi_t^* w)] \Big|_{s=0} = \frac{d}{du} [\phi_u^* w] \Big|_{u=t}.$$

If we choose f as an observable function $f = G$

$$\frac{d}{dt} (\phi_t^* G) = \phi_t^* (X_H G) = \phi_t^* \{G, H\},$$

by integrating both sides from 0 to T we obtain

$$\frac{1}{T} [G \circ \phi_T - G] = \frac{1}{T} \int_0^T \{G, H\} \circ \phi_t dt.$$

If the function remains bounded in its time evolution, taking the limit when T goes to infinity

$$\langle \langle \{G, H\} \rangle \rangle = 0.$$

As an instance, when $M = T^*\mathbb{R}^3$ and $G = \mathbf{x} \cdot \mathbf{p}$ we obtain

$$X_G = \sum_{i=1}^3 \left(x^i \frac{\partial}{\partial x^i} - p_i \frac{\partial}{\partial p_i} \right).$$

If the Hamiltonian is given by

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m} \mathbf{p} \cdot \mathbf{p} + V(\mathbf{x}) = K(\mathbf{p}) + V(\mathbf{x}),$$

then

$$X_G H = -2K + \mathbf{x} \cdot \nabla V.$$

Thus, taking the limit of T going to infinity we obtain

$$\langle\langle 2K \rangle\rangle = \langle\langle \mathbf{x} \cdot \nabla V \rangle\rangle .$$

2.1 Virial theorem for Henon–Heiles system

The Hamiltonian of the Henon–Heiles system is given by

$$H = \frac{1}{2}(p_x^2 + p_y^2 + ax^2 + by^2) + dx^2y - \frac{1}{3}ey^3 .$$

Three known integrable cases were found by the Painlevé method in [7], Fordy [8] employed the technique connecting the Hamiltonian formalisms of stationary and nonstationary flows to prove that these were the only three integrable cases of the system

- $d/e = -1, a = b$.
- $d/e = -1/6, a, b$ arbitrary.
- $d/e = -1/16, b = 16a$ arbitrary.

The bi-Hamiltonian properties have been exhibited only for the first case where the additional first integral is given by

$$H_2 = \left(xy + x^2y + \frac{1}{3}y^3 + p_x p_y \right)$$

and other two cases do not have a second first integral.

The virial function

$$G = xp_x + yp_y$$

yields

$$\dot{G} = p_x \frac{\partial H}{\partial p_x} + p_y \frac{\partial H}{\partial p_y} - x \frac{\partial H}{\partial x} - y \frac{\partial H}{\partial y} = 2K - \mathbf{x} \cdot \nabla H .$$

Thus, we obtain classical VT

$$2 \langle\langle K \rangle\rangle = \langle\langle \mathbf{x} \cdot \nabla H \rangle\rangle .$$

From energy conservation $\langle\langle K \rangle\rangle + \langle\langle V \rangle\rangle = E$ we obtain

$$2E = \left\langle\left\langle 2ax^2 + 2by^2 + 5dx^2y - \frac{5}{3}ey^3 \right\rangle\right\rangle = \langle\langle \mathcal{P}(x, y) \rangle\rangle .$$

The asymptotic invariant polynomial $\mathcal{P}(x, y)$ converges rapidly to $2E$ in both regular and chaotic cases; the only apparent difference between the regular and chaotic cases is the somewhat larger oscillations in the latter case. The convergence of the virial integrals for chaotic orbits is complicated by sticky regions, where an orbit can spend long intervals exploring islands [9].

3. Conformal Hamiltonian systems and virial theorem

Let (M, ω) be a symplectic manifold, where M is a differentiable manifold endowed with a symplectic form ω . Consider a diffeomorphism ϕ such that $\phi^*(\omega) = k\omega$, where $0 \neq k \in \mathbb{R}$ are called non-strictly canonical transformations. Let the vector field Γ be the generator of a one-parameter group of non-strictly canonical transformations $\phi_\epsilon^*(\omega) = k(\epsilon)\omega$. Then, there exists a real number $a \neq 0$ such that Lie derivative of the dynamical vector field Γ satisfies $L_\Gamma \omega = a\omega$, with k and a related by $k(\epsilon) = \exp(a\epsilon)$. Note that, in [5] a dynamics given by a Hamiltonian vector field and a non-strictly canonical infinitesimal symmetry were considered. In this study, we are considering the dynamics given by a non-Hamiltonian vector field and also a Hamiltonian vector field X . Procedures are different but the result is almost the same.

If $\pi: E \rightarrow Q$ is a vector bundle, the vector field generating dilation along the fibres is well defined: $v(\partial/\partial v)$ if $E = TQ$ or $p(\partial/\partial p)$ if $E = T^*Q$. When $E = T^*\mathbb{R}$, the vector field

$$X_G = -\frac{1}{2} \sum_{i=1}^n \left(q_i \frac{\partial}{\partial q_i} + p_i \frac{\partial}{\partial p_i} \right)$$

generates dilations in identifying $T^*\mathbb{R} \simeq \mathbb{R} \oplus \mathbb{R}$. One must note that X_G is not a Hamiltonian operator. Its action on the symplectic form $\omega = \sum_{i=1}^n dq^i \wedge dp_i$ gives $\mathcal{L}_{X_G} \omega = -\omega$.

However, if Γ satisfies $\mathcal{L}_\Gamma \omega = a\omega$, then $aX_G + \Gamma$ is a locally-Hamiltonian vector field because

$$\mathcal{L}_{aX_G + \Gamma}(\omega) = 0.$$

Let $\Gamma = X_f - aX_G$, then the action of X on the Hamiltonian is given by

$$\Gamma(H) = \{H, f\} - aX_G(H).$$

If we assume that $H = K(p) + V(q)$, we find

$$X_G(H) = -\frac{1}{2} \left(2K(p) + \sum_{i=1}^n q^i \frac{\partial H}{\partial q^i} \right).$$

In this case, the virial expression is given by

$$2a \langle \langle K \rangle \rangle = \langle \langle \Gamma(H) \rangle \rangle.$$

3.1 Application to Gierer–Meinhardt system

The dynamical vector field of the autocatalytic Gierer–Meinhardt (GM) system [10] satisfies $L_\Gamma \omega = (c+h)\omega$. Hence the flow Γ is made of non-strictly canonical transformations with valence $e^{(c+h)t}$. When we impose $c+h=0$, Γ becomes symplectic or Hamiltonian vector field. When restricted to the symplectic case, i.e., $c=-h$, the associated Hamiltonian is given by

$$H = a \log(b+y) - D \frac{x^2}{2} - cxy$$

with standard Poisson brackets $\{x, y\} = 1$ and equations of motion are given by

$$\dot{x} = \{x, H\} = \frac{\partial H}{\partial y} = \frac{a}{b+y} - cx,$$

$$\dot{y} = \{y, H\} = -\frac{\partial H}{\partial x} = Dx + cy.$$

When the manifold is \mathbb{R}^2 with coordinates (x, y) and $\omega = dx \wedge dy$, the vector fields whose flow is made of non-strictly canonical transformations are

$$\dot{x} = \frac{\partial H}{\partial y}, \quad \dot{y} = -\frac{\partial H}{\partial x} + \kappa y,$$

where $H: \mathbb{R}^2 \rightarrow \mathbb{R}$ is the Hamiltonian. The flow has the property $\phi^* \omega = e^{\kappa t} \omega$, and so the symplectic inner product of any two tangent vectors contracts exponentially if $\kappa < 0$. If ω is a locally symplectic structure (LCS) then the two LCS ω and $\omega' = e^{\kappa t} \omega$ are conformally equivalent [11].

Thus, the general activator–inhibitor system can be expressed as

$$\dot{x} = \frac{\partial H}{\partial y}, \quad \dot{y} = -\frac{\partial H}{\partial x} - (c+h)y.$$

Given $H \in C^\infty(M)$, the vector field Γ (or X_H^c – usual notation) satisfies

$$i_{X_H^c} \omega = dH - (c+h)\theta, \quad \theta = y dx.$$

The conformal vector field is given by $X_H + (c+h)Z$, where Z is defined by $i_Z \omega = -\theta$. So, it turns out that $Z = y \partial_y$.

4. Virial theorem and the Liénard II system

Given a second-order ordinary differential equation (ODE)

$$\ddot{x} = \mathcal{F}(x, \dot{x}), \tag{1}$$

we define the Jacobi last multiplier (JLM) M as a solution of the following ODE:

$$\frac{d \log M}{dt} + \frac{\partial \mathcal{F}(x, \dot{x})}{\partial \dot{x}} = 0. \tag{2}$$

In fact, as the dynamical vector field for (1) is

$$\Gamma = \dot{x} \frac{\partial}{\partial x} + \mathcal{F} \frac{\partial}{\partial \dot{x}}$$

then $\text{div } \Gamma = \partial \mathcal{F} / \partial \dot{x}$ and (2) is the JLM equation (e.g., see [12,13]).

Assuming (1) to be derivable from the Euler–Lagrange equation of a Lagrangian L , one can show that the JLM is related to the Lagrangian by the following equation:

$$M = \frac{\partial^2 L}{\partial \dot{x}^2}. \tag{3}$$

Moreover, in each JLM, M defines in an essentially unique way (i.e., up to addition of a gauge term) a Lagrangian such that (3) holds.

Virial theorem for the Liénard-type systems

In case of the Liénard II equation

$$\ddot{x} + f(x)\dot{x}^2 + g(x) = 0, \quad (4)$$

where $\mathcal{F} = -f(x)v^2 - g(x)$, and one can show that the solution of the JLM is given by

$$M(x) = e^{2F(x)}, \quad F(x) := \int^x f(s)ds. \quad (5)$$

Furthermore, it follows from (3) that its Lagrangian is

$$L(x, \dot{x}) = \frac{1}{2}e^{2F(x)}\dot{x}^2 - V(x), \quad (6)$$

where the potential term

$$V(x) = \int^x e^{2F(s)}g(s)ds. \quad (7)$$

The image under the Legendre transformation yields the conjugate momentum

$$p := \frac{\partial L}{\partial \dot{x}} = \dot{x}e^{2F(x)} \text{ implies } \dot{x} = pe^{-2F(x)}, \quad (8)$$

so that the final expression for the Hamiltonian is

$$H = \frac{p^2}{2M(x)} + \int^x M(s)g(s)ds, \quad (9)$$

where it is explicitly denoted in terms of the last multiplier $M(x)$ to highlight its role as a position-dependent mass term [14].

4.1 Another virial theorem

Given a differentiable function L on TQ we can construct a semibasic one-form $\theta_L \in \wedge^1(TQ)$ and an exact two-form $\omega_L \in \wedge^2(TQ)$, given by

$$\theta_L = S^*(dL), \quad \omega_L = -d\theta_L,$$

where S is the vertical endomorphism. The Lagrangian L is said to be regular, then ω_L is symplectic. The energy function is

$$E_L = \Delta(L) - L, \quad \Delta = \text{Liouville vector field.}$$

The dynamics is given by the vector field $X_L \in \mathfrak{X}(TQ)$ such that $i(X_L)\omega_L = dE_L$.

If a vector field $X \in \mathfrak{X}(TQ)$ is the complete lift of a vector field $Y \in \mathfrak{X}(Q)$, then

$$\mathcal{L}_X\theta_L = \theta_{X(L)}, \quad X(E_L) = E_{X(L)}.$$

Let Y be the vector field in \mathbb{R} given by

$$Y = \xi(x) \frac{\partial}{\partial x},$$

whose complete lift is given by

$$X(x, \dot{x}) = Y^c(x, \dot{x}) = \xi(x)\partial_x + \xi_x\dot{x}\partial_{\dot{x}}.$$

When the vector field Y is such that

$$X(L) = Y^c(L) = aL, \quad a \in \mathbb{R} \tag{10}$$

then

$$\mathcal{L}_X \omega_L = a\omega_L \quad \text{and} \quad \mathcal{L}_X E_L = aE_L.$$

Such a vector field X is a symmetry of the dynamical vector X_L , i.e.,

$$[X, X_L] = 0.$$

The important point is that the function $G = i(X)\theta_L$ is such that $X_L(G) = aL$ and therefore we obtain the virial type result $\langle\langle L \rangle\rangle = 0$. In the particular case of a position-dependent mass Lagrangian

$$L(x, v) = \frac{1}{2}m(x)v^2 - V(x)$$

the condition $X(L) = aL$ implies that the unknown functions ξ and the potential $V(x)$ are to be determined from the following relations:

$$\xi'(x) + \frac{m'(x)}{2m(x)}\xi(x) = \frac{a}{2}, \tag{11}$$

$$\xi(x)V'(x) = aV(x). \tag{12}$$

As an example, we consider the vector field X that is the complete lift of the vector field Y generating the dilations in $Q = \mathbb{R}^3$, given by

$$X = Y^c = \sum_{i=1}^3 \left(x^i \frac{\partial}{\partial x^i} + v^i \frac{\partial}{\partial v^i} \right),$$

and the Lagrangian of a harmonic oscillator with $k = m$, $L = \frac{1}{2}m\mathbf{v} \cdot \mathbf{v} - \frac{1}{2}m\mathbf{x} \cdot \mathbf{x}$. Here $\theta_L(x, v) = mv \, dx$, then $\omega_L = m \, dx \wedge dv$ and the energy function is $E_L = \frac{1}{2}m(v^2 + x^2)$. Therefore,

$$X_L = v \frac{\partial}{\partial x} - x \frac{\partial}{\partial v},$$

and consequently $G = mxv$, $X(L)$ being

$$X(L) = X \left(\frac{1}{2}m\mathbf{v} \cdot \mathbf{v} - \frac{1}{2}m\mathbf{x} \cdot \mathbf{x} \right) = 2L,$$

i.e., the particular case $a = 2$. One can also check

$$[X, X_L] = \left[x \frac{\partial}{\partial x} + v \frac{\partial}{\partial v}, v \frac{\partial}{\partial x} - x \frac{\partial}{\partial v} \right] = 0.$$

Thus VT provides $\langle\langle X_L G \rangle\rangle = 2 \langle\langle L \rangle\rangle = 0$.

Liénard-type equation. When

$$X_L = v \frac{\partial}{\partial x} - (f(x)v + g(x)) \frac{\partial}{\partial v}$$

operates on $G = m(x)\xi(x)v$ for Liénard II equation it yields eqs (11) and (12), where $V'(x)/m(x) = g(x)$.

We can determine $\xi(x)$ from (11) to be

$$\xi(x) = \frac{1}{\sqrt{m(x)}} \left(C_1 + \frac{a}{2} \int_0^x \sqrt{m(s)} ds \right). \quad (13)$$

Using this expression, the potential turns out to be

$$V(x) = C_2 \exp \left(a \int_0^x \frac{ds}{\xi(s)} \right). \quad (14)$$

5. Virial theorem in quantum world

Let \mathcal{H} be the complexified Hilbert space of Lebesgue integrable functions on \mathbb{R}^3 with Hermitian inner product

$$\langle u_1, u_2 \rangle = \int d^3x u_2(\mathbf{x}) \bar{u}_1(\mathbf{x}).$$

The realification of the Hilbert space \mathcal{H} (real Banach manifold) is endowed with a natural symplectic structure

$$\omega(u, v) = 2 \operatorname{Im} \langle u, v \rangle.$$

Given a self-adjoint linear operator \hat{H} we can define a real function h in \mathcal{H} by

$$h(u) = \langle u, \hat{H}u \rangle.$$

Then

$$\begin{aligned} dh(u)(v) &= d \langle u, \hat{H}u \rangle(v) \\ &= \left. \frac{d}{ds} \right|_{s=0} \langle u + sv, \hat{H}(u + sv) \rangle \\ &= \left. \frac{d}{ds} \right|_{s=0} (\langle u, \hat{H}u \rangle + s \langle u, \hat{H}v \rangle + s \langle v, \hat{H}u \rangle + s^2 \langle v, \hat{H}v \rangle) \\ &= (\langle u, \hat{H}v \rangle + \langle v, \hat{H}u \rangle) = 2 \langle u, \hat{H}v \rangle \\ &= 2i \langle u, -i \hat{H}v \rangle = \omega(u, -i \hat{H}v). \end{aligned}$$

Therefore, if \hat{H} is the Hamiltonian of a quantum system, the Schrödinger equation describing time evolution plays the role of Hamiltonian equations for the Hamiltonian dynamical system (\mathcal{H}, ω, h) , where $h(u) = \langle u, \hat{H}u \rangle$, the integral curves of X_h satisfy

$$\dot{u} = X_h(u) = -i \hat{H}u.$$

Thus $h(u)$ and $-i \hat{H}$ stand for Hamiltonian and Hamiltonian vector field for the quantum system.

Let us consider two Hamiltonian functions $f(u) = \langle u, \hat{F}u \rangle$ and $g(u) = \langle u, \hat{G}u \rangle$ corresponding to two self-adjoint operators \hat{F} and \hat{G} .

$$\begin{aligned} \{f, g\}(u) &= \omega(X_f, X_g)(u) = 2 \operatorname{Im} \langle \hat{F}u, \hat{G}u \rangle \\ &= -i [\langle \hat{F}u, \hat{G}u \rangle - \langle \hat{G}u, \hat{F}u \rangle] \\ &= -i [\langle u, \hat{F}\hat{G}u \rangle - \langle u, \hat{G}\hat{F}u \rangle] \\ &= -i [\langle u, [\hat{F}, \hat{G}]u \rangle]. \end{aligned}$$

The integral curves of the vector field X_h yields

$$\dot{a}(u) = \{a, h\}(u) = -i \langle u, [\hat{A}, \hat{H}]u \rangle$$

and Ehrenfest theorem

$$\frac{d}{dt} \langle u, \hat{A}u \rangle = -i \langle u, [\hat{A}, \hat{H}]u \rangle.$$

If we integrate between 0 and T we obtain

$$\langle u(T), \hat{A}u(T) \rangle - \langle u(0), \hat{A}u(0) \rangle = -i \int_0^T \langle u, [\hat{A}, \hat{H}]u \rangle dt,$$

and if $\langle u, [\hat{A}, \hat{H}]u \rangle$ remains bounded then taking the limit for $T \rightarrow \infty$ of the quotient of both sides by T yields the quantum VT

$$\overline{\langle u, [\hat{A}, \hat{H}]u \rangle} = 0.$$

Suppose that the Hamiltonian of a quantum system is

$$H = \frac{1}{2} \hat{\mathbf{p}} \cdot \hat{\mathbf{p}} + V(\mathbf{x}), \text{ where } \hat{\mathbf{p}} = -i \nabla.$$

Let G be given by

$$G = \frac{1}{2} (\hat{\mathbf{p}} \cdot \mathbf{x} + \mathbf{x} \cdot \hat{\mathbf{p}}),$$

then we obtain the *standard quantum virial*

$$\overline{\langle u, \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}u \rangle} - \overline{\langle u, (\mathbf{x} \cdot \nabla V(\mathbf{x}))u \rangle} = 0.$$

5.1 Application to quantum Liénard II

In this section, we apply the scheme to quantum Liénard II equation [15]. It has been shown in [16] that the appropriate Hilbert space for the description of position-dependent mass systems is $\mathcal{H} = L^2(\mathbb{R}, d\mu)$ with $d\mu = \sqrt{m(x)} dx$. Here $(d\mu/dx) = \sqrt{m(x)}(\partial/\partial x)$, is the (square root of the) Radon–Nikodym derivative [17] of the measure $d\mu$ with respect to the Lebesgue measure dx .

Let us recall few basic definitions. Let (X, \mathcal{F}) be a measure space and m be a non-negative Borel function. Note that

$$\mu(E) = \int_E m dv, \quad E \in \mathcal{F}$$

is a measure satisfying $\nu(E) = 0$ implies $\mu(E) = 0$. We say μ is absolutely continuous with respect to ν and the function f is called the Radon–Nikodym derivative or density of μ with respect to ν and is denoted by $d\mu/d\nu$.

Symplectomorphism and Radon–Nikodym derivative. The momentum of the Liénard II is given by

$$p_\mu = \frac{P_x}{\sqrt{M(x)}} \quad \mu = \mu(x).$$

Virial theorem for the Liénard-type systems

The transformation (p_x, x) to (p_μ, μ) satisfies

$$p_x dx = p_\mu d\mu \quad \text{or} \quad dp_x \wedge dx = dp_\mu \wedge d\mu.$$

The important point is that there are no translations on the measure.

If $d\mu = \sqrt{M(x)}dx$ is a measure then the norm of the function ψ is given by

$$\|\psi\|^2 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \sqrt{M(x)} dx.$$

The Hamiltonian operator is given by

$$\hat{H} = K + V = \frac{1}{2}\hat{p}^2 + V(x), \quad \hat{p} = -\frac{i}{\sqrt{M(x)}} \frac{\partial}{\partial x}.$$

We illustrate our construction using the free particle motion of the Mathews–Lakshmanan system [18] characterized by

$$L(x, v, \lambda) = \frac{1}{2} \left(\frac{v^2}{1 + \lambda x^2} \right).$$

The Lagrangian function is invariant under the action of the vector field $X = \sqrt{1 + \lambda x^2} (\partial/\partial x)$ such that the complete lift

$$X^c = \sqrt{1 + \lambda x^2} \frac{\partial}{\partial x} + \left(\frac{\lambda x v}{\sqrt{1 + \lambda x^2}} \right) \frac{\partial}{\partial v}$$

satisfies $X^c(L) = 0$. This vector field can be seen as a Killing vector field for the metric $g = (1 + \lambda x^2)^{-1} dx^2$. It is clear that the natural measure in the real line is not invariant under such vector fields; instead, the only invariant measures are the multiples

$$d\mu = \frac{1}{\sqrt{1 + \lambda x^2}} dx.$$

Thus the multiplier is $M(x) = (1 + \lambda x^2)^{-1}$.

In order to apply the VT we introduce the generator of the dilation $\hat{G} = \xi(x)(\partial/\partial x)$ with the property

$$[\hat{p}, \hat{G}] = \frac{a}{2} \hat{p}.$$

The general solution of $\xi(x)$ is given by

$$\xi(x) = \frac{1}{\sqrt{M(x)}} \left(c_1 + \frac{a}{2} \int_0^x \sqrt{M(\zeta)} d\zeta \right).$$

6. Discussion and outlook

All the classical cases discussed in this paper are finite-dimensional in nature. This can be generalized to infinite-dimensional framework. In 1970, Vlasov *et al* [19] proved that solutions of nonlinear Schrödinger equation

$$iu_t(x_1, x_2, t) + \frac{1}{2} \nabla u + |u|^2 u = 0, \quad u(x_1, x_2, t) = u_0(x_1, x_2)$$

satisfy the so-called virial theorem (also called variance identity), given by

$$\frac{d^2}{dt^2} \mathcal{F}(t) \equiv \frac{d^2}{dt^2} \int (x_1^2 + x_2^2) |u|^2 d\mathbf{x} = 4E, \quad E = \frac{1}{2} \int (|\nabla u_0|^2 |u_0|^4) d\mathbf{x}.$$

We can derive this relation using the following quadratic form associated with a self-adjoint differential operator of first-order:

$$\begin{aligned} F(t) &= \frac{1}{2} (\omega(Au, u) - \omega(u, Au)) = i \int_{\mathbb{R}^n} x_j (u \partial_{x_j} u^* - u^* \partial_{x_j} u) d\mathbf{x} \\ &= \frac{d}{dt} \int_{\mathbb{R}^n} x_j^2 |u(x, t)|^2 d\mathbf{x} = \frac{d}{dt} \mathcal{F}(t), \end{aligned}$$

where we have used

$$i \partial_t u = -\frac{1}{2} \Delta u + \beta |u|^{2\sigma} u.$$

If we differentiate $F(t)$ we obtain

$$\begin{aligned} \frac{d^2}{dt^2} \mathcal{F}(t) &= \frac{dF}{dt} = i \int_{\mathbb{R}^n} x_j (\partial_t u \partial_{x_j} u^* + u \partial_t \partial_{x_j} u^* - \partial_t u^* \partial_{x_j} u - u^* \partial_t \partial_{x_j} u) d\mathbf{x} \\ &= i \int_{\mathbb{R}^n} \left(2x_j (\partial_t u \partial_{x_j} u^* - \partial_t u^* \partial_{x_j} u) + (u^* \partial_t u - u \partial_t u^*) \right) d\mathbf{x} \\ &= \int_{\mathbb{R}^n} \left(2|\partial_{x_j} u|^2 + \frac{2\sigma\beta}{\sigma+1} |u|^{2\sigma+2} - 2x_j |u|^2 \partial_{x_j} V(x) \right) d\mathbf{x}. \end{aligned}$$

Using the nonlinear Schrödinger equation we obtain

$$\frac{dF}{dt} = 4E + \frac{2\beta(n\sigma - 2)}{\sigma + 1} \int_{\mathbb{R}^n} |u|^{2\sigma+2} d\mathbf{x},$$

and at the critical dimension $dn = 2$ this reduces to

$$\frac{dF}{dt} = 4E.$$

Under the NLSE flow $F(u)$ and (dF/dt) are called Morawetz and virial identity. The term virial identity comes from the analogy to the virial theorem in classical mechanics (for a rigorous proof, see [20]).

In this paper, we have given a brief outline of the application of the generalized virial theorem. It would be interesting to study the virial theorem associated with Riemannian manifolds and other Hamiltonian partial differential equations.

Acknowledgements

The authors are extremely thankful and grateful to other collaborators, Manuel F Rañada, Fernando Falceto and Irina Gheorghiu, in this project for their valuable discussions. Authors are also grateful to referee for the comments and valuable suggestions. Partial financial support by the research projects MTMØ2012/33575 (MINECO, Madrid) and DGA-E24/1 (DGA, Zaragoza) is acknowledged. Finally, and most importantly, PG acknowledges the efficient, friendly, considerate and professional assistance he received from the organizing members of the PNLD 2013 meeting.

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